NASA Advanced Computing Environment for Science & Engineering

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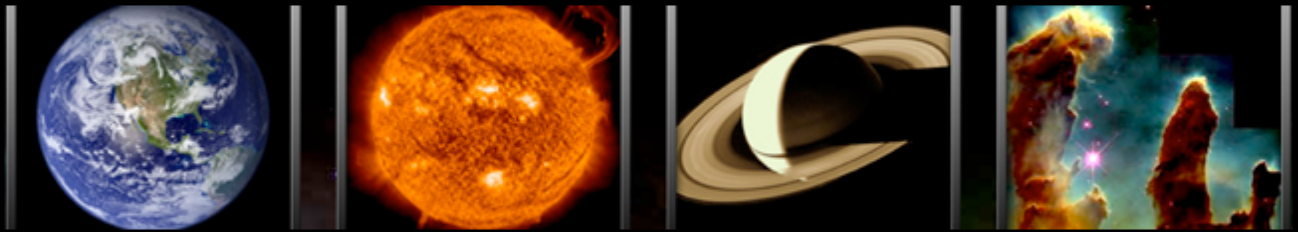
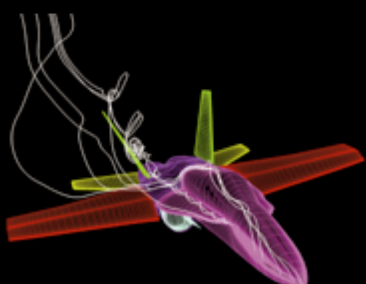
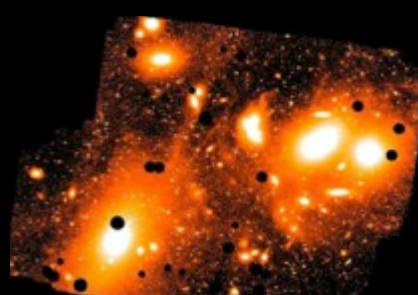
NASA Overview: Mission Directorates

- **Vision:** *To reach for new heights and reveal the unknown so that what we do and learn will benefit all humankind*
- **Mission:** *To pioneer the future in space exploration, scientific discovery, and aeronautics research*
- **Aeronautics Research (ARMD):** Pioneer and prove new flight technologies for safer, more secure, efficient, and environmentally friendly air transportation
- **Human Exploration and Operations (HEOMD):** Focus on ISS operations; and develop new spacecraft and other capabilities for affordable, sustainable exploration beyond low Earth orbit
- **Science (SCMD):** Explore the Earth, solar system, and universe beyond; chart best route for discovery; and reap the benefits of Earth and space exploration for society
- **Space Technology (STMD):** Rapidly develop, demonstrate, and infuse revolutionary, high-payoff technologies through collaborative partnerships, expanding the boundaries of aerospace enterprise



NASA Overview: Centers & Facilities

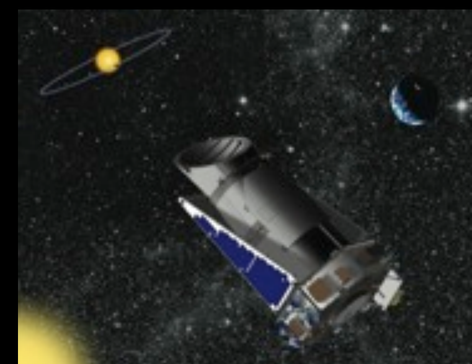




Need for Advanced Computing

Enables modeling, simulation, analysis, and decision-making

- Digital experiments and physical experiments are tradable
- Physical systems and live tests are generally expensive & dangerous (e.g., extreme environments), require long wait times, and offer limited sensor data
- NASA collects and curates vast amounts of observational science data that require extensive analysis and innovative analytics to advance our understanding

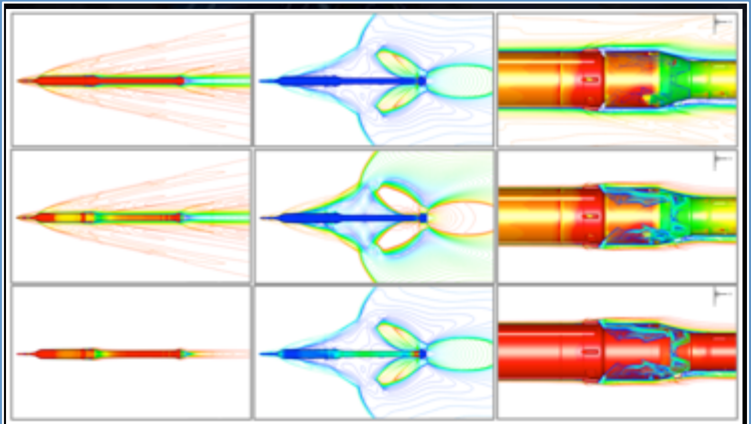


- Decades of exponentially advancing computing technology has enabled dramatic improvements in cost, speed, and accuracy – in addition to providing a predictive capability
- Many problems pose extremely difficult combinatorial optimization challenges that can only be solved accurately using advanced technologies such as quantum computing
- NASA's goals in aeronautics, Earth and space sciences, and human and robotic exploration all require orders-of-magnitude increase in computing capability to enhance accuracy, reduce cost, mitigate risk, accelerate R&D, and heighten societal impact

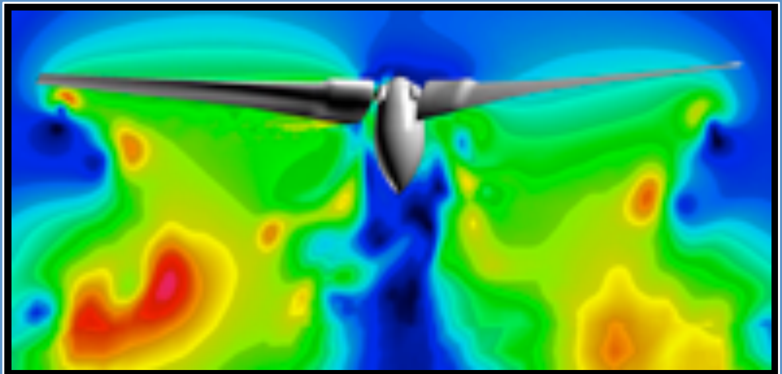
Advanced Computing Environment

NASA's Diverse HPC Requirements

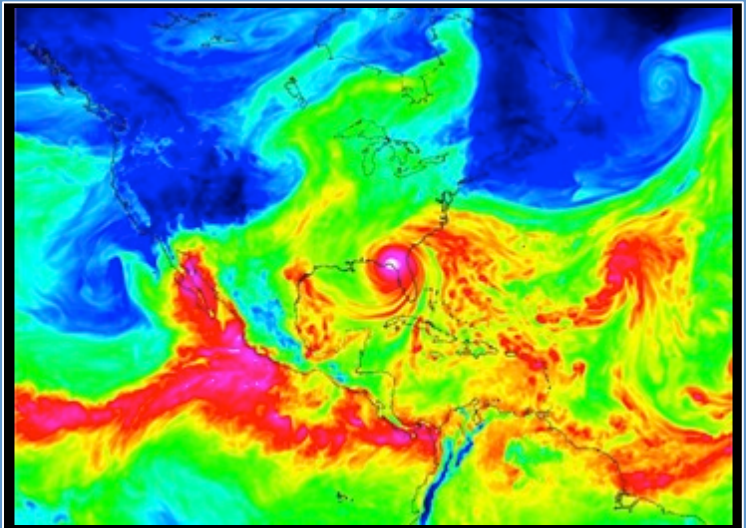
- Engineering requires HPC resources that can process large ensembles of moderate-scale computations to efficiently explore design space ***(high throughput / capacity)***
- Research requires HPC resources that can handle high-fidelity long-running large-scale computations to advance theoretical understanding ***(leadership / capability)***



Aerodynamic database generation



Rotary wing unsteady aerodynamics



Real-time hurricane prediction

- Time-sensitive mission-critical applications require HPC resources on demand ***(high availability / maintain readiness)***

Balanced HPC Environment

Computing Systems

- ***Pleiades:*** 212K-core SGI Altix ICE with 4 generations of Intel Xeon (4 racks GPU-enhanced: M2090, K40; 16 nodes have Phi 5110P); 723 TB RAM; 5.3 PF peak
- ***Merope:*** 12K-core SGI Altix ICE with 2 generations of Intel Xeon; 28 TB RAM; 141 TF peak
- ***Endeavour:*** Two SGI UV2000 nodes with 2 and 4 TB shared memory SSI via NUMALink-6; 32 TF peak
- ***hyperwall:*** 1024-core AMD Opteron, 128-node GPU M2090 cluster for large-scale rendering & concurrent visualization

Data Storage

- 20 PB of RAID over several Lustre filesystems
- 115 PB of tape archive

Networks

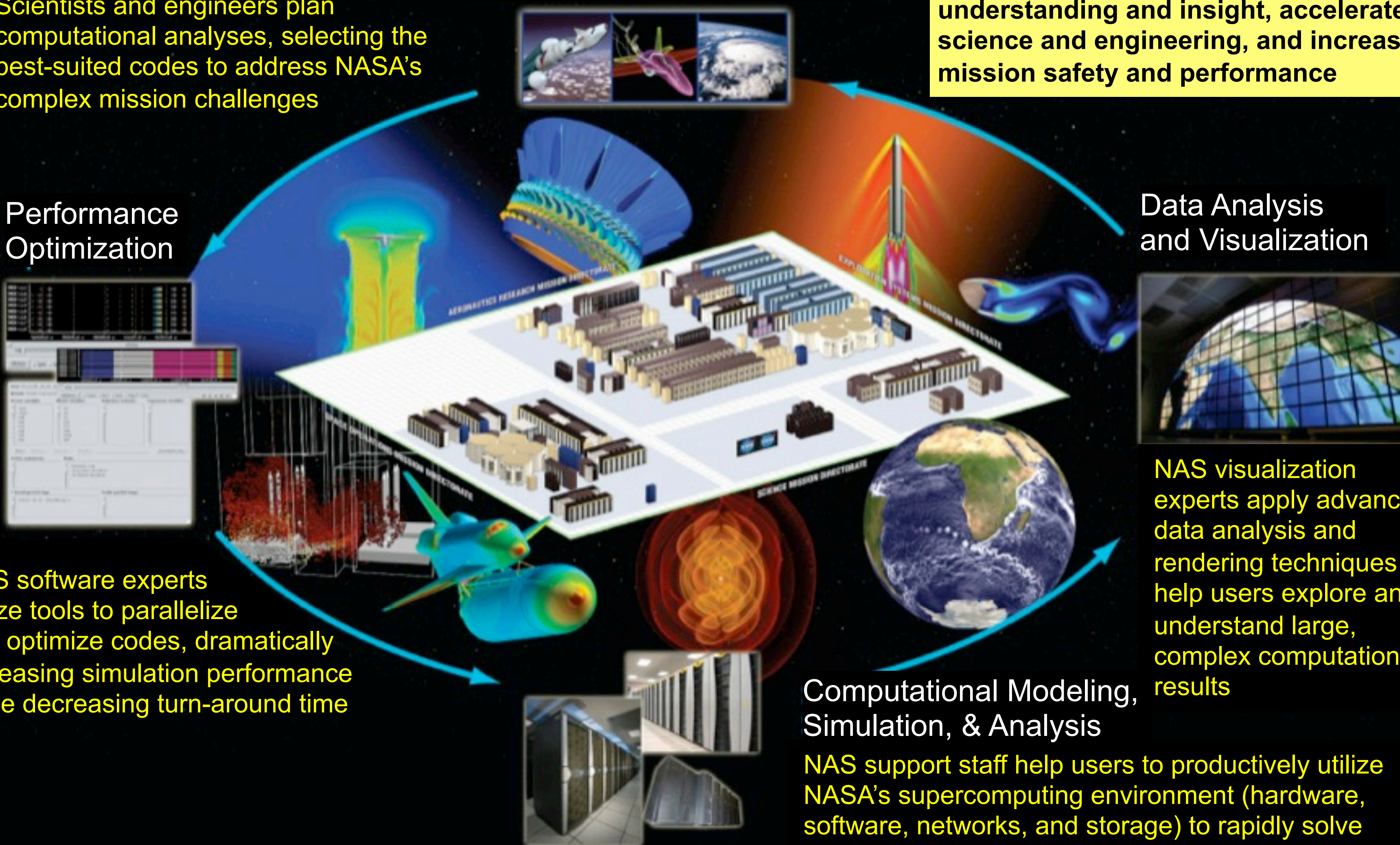
- InfiniBand interconnect for Pleiades in partial hypercube topology; connects all other HPC components as well
- 10 Gb/s external peering

Integrated Spiral Support Services

Outcome: Dramatically enhanced understanding and insight, accelerated science and engineering, and increased mission safety and performance

NASA Mission Challenges

Scientists and engineers plan computational analyses, selecting the best-suited codes to address NASA's complex mission challenges



Performance Optimization

NAS software experts utilize tools to parallelize and optimize codes, dramatically increasing simulation performance while decreasing turn-around time

Data Analysis and Visualization

NAS visualization experts apply advanced data analysis and rendering techniques to help users explore and understand large, complex computational results

Computational Modeling, Simulation, & Analysis

NAS support staff help users to productively utilize NASA's supercomputing environment (hardware, software, networks, and storage) to rapidly solve large computational problems

Accelerator Technologies

Significant performance potential for science and engineering applications

- Execute many threads simultaneously at relatively lower power

Two primary viable options

- ***<u>Nvidia GPGPU</u>:*** Did not get much traction within NASA
- ***<u>Intel MIC</u>:*** Code commonality across host and co-processor was initially promising

Intel Xeon Phi (KNC) evaluation

- 128 nodes, each with 2 Sandy Bridge and 2 KNC
- Examine performance in four different execution modes: Native Host, Off-load, Symmetric, Native MIC
- *Micro-kernel benchmarks:* Memory bandwidth / latency, MPI functions, OpenMP constructs
- *NAS Parallel Benchmarks (NPB):* OpenMP, MPI, MPI+OpenMP
- *Applications:* OVERFLOW, Cart3D, WRF
- Results reported without extensive code modifications

Summary Performance Results

- System stability initially an issue but situation improved as MPSS (Many-core Platform Software Stack) has matured
- Running codes in Native modes lead to wasted resources
- MPI and OpenMP overhead very high on MIC compared to on host
- Off-load mode has significant overhead associated with data transfer
- Optimal load balancing in Symmetric mode is extremely challenging
- Hybrid code in Symmetric mode yields best performance due to reduced MPI communication and improved resource utilization
- Obtaining good performance on KNC is not simple – requires careful design of data structure and memory layout, and lots of parallelism
- KNC not ready for prime time, but next generation KNL looks promising due to no host and several other architectural improvements

- Extensive details in SC2013 paper by S. Saini et al.: *"An early performance evaluation of many integrated core architecture based SGI rackable computing system"*

Big Data

NASA has enormous collections of observational and model data

- <u>Observational Data</u>
  - Tens of satellites and telescopes producing multi-petabytes of data per year
  - SMD's Earth Science Division operates 12 DAACs (archive centers) containing ~10 PB of data
  - Solar Dynamics Observatory (SDO) satellite produces 1 GB per minute; translates to ~3 PB over its 5-year life cycle
- <u>Model / Simulation Data</u>
  - NAS Division has 20 PB of unique data in global filesystems and 115 PB of archive storage
  - MITgcm code running at 1/48th degree resolution on 35K cores produced 1.4 PB during its 5-day run; full simulation will produce 9–18 PB

DISE (Data Intensive Supercomputing Environment) integrates Big Data and Big Compute to support analysis and analytics of NASA data

Fun Fact: The term "Big Data" was first used by Michael Cox & David Ellsworth of NAS Division in a Visualization '97 paper: *"Visualizing flow around an airframe"*, where largest dataset considered was 7.5 GB

Big Data Challenges for Users

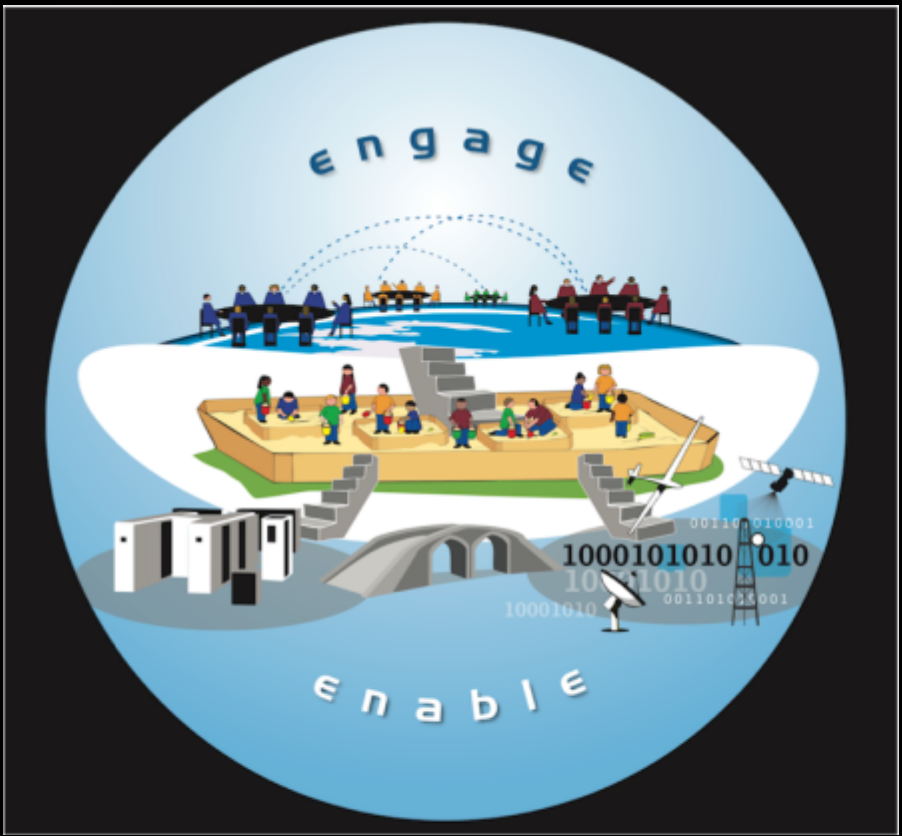
Conducted survey of NASA projects dealing with Big Data to gather user requirements

Developing a roadmap including prototype implementations

- ***Data Discovery:*** Finding what data is available and where
- ***Data Management:*** Transferring very large datasets from archives to computational resources
- ***Tools / Models / Algorithms:*** Developing analysis & analytics software at scale
- ***Analysis Workflow:*** Handling increasingly complex processing pipelines
- ***Analysis / Analytics Infrastructure:*** Dealing with inadequacy of available heterogeneous resources
- ***Collaboration Environments:*** Difficulty with sharing knowledge across a wider community

NASA Earth Exchange (NEX)

A collaborative environment that brings scientists and researchers together in a knowledge-based social network along with observational data, tools, and computing power to provide transparency and accelerate research



VISION

To provide "*Science as a Service*" to the Earth science community addressing global environmental challenges

GOAL

To improve efficiency and expand the scope of NASA Earth science technology, research, and applications programs

NEX Environment

Collaboration Portal (over 400 members)

Tools, Models, Workflows, Papers, Data

Compute Resources (over 5 PF computing)

Sandbox for experimentation, HPC (Pleiades)

Data Repository (over 2 PB of data)

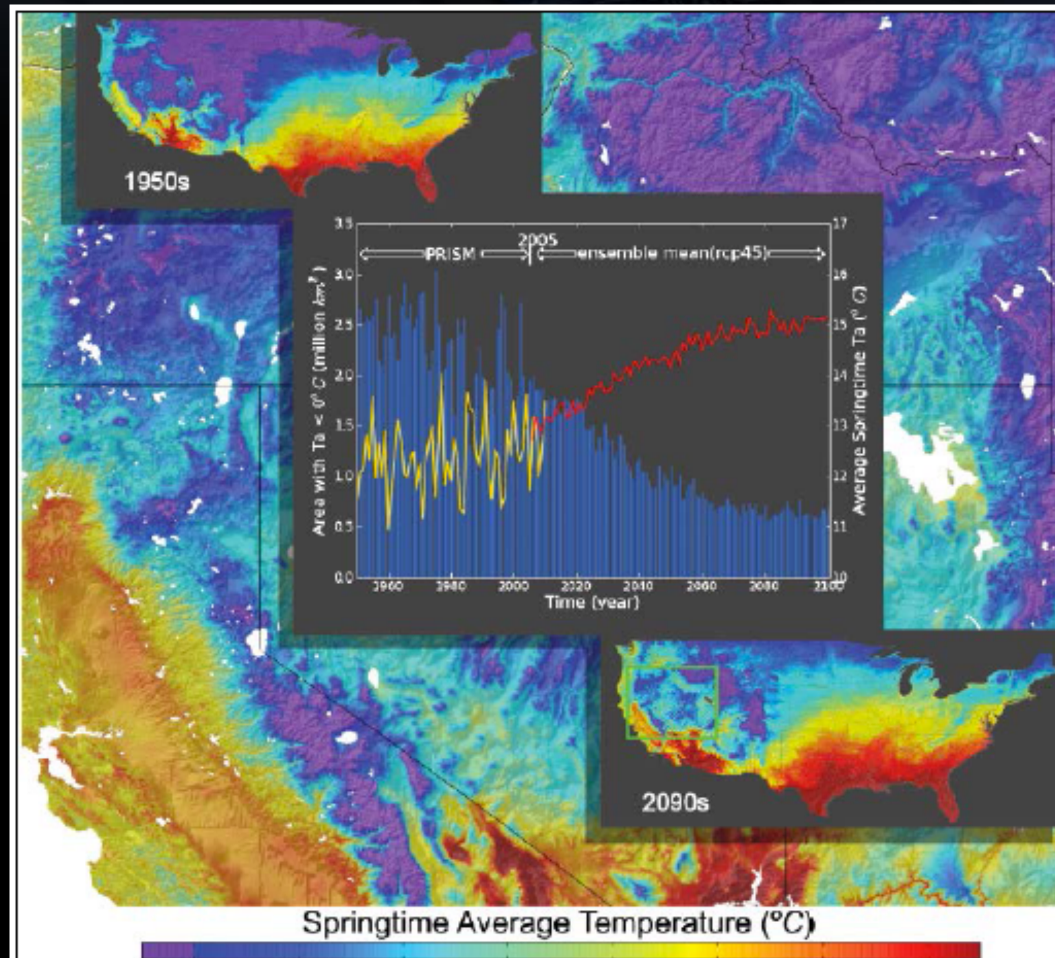
Working copies of Observational and Project data

- Collaboration portal open to all Earth scientists
- Sandbox currently available to a subset of scientists with NASA credentials
- HPC resources available only to approved projects with allocation
- OpenNEX, a collaboration with Amazon, provides NEX datasets to the wider Earth science community

High-Resolution Climate Projections

National Climate Assessment

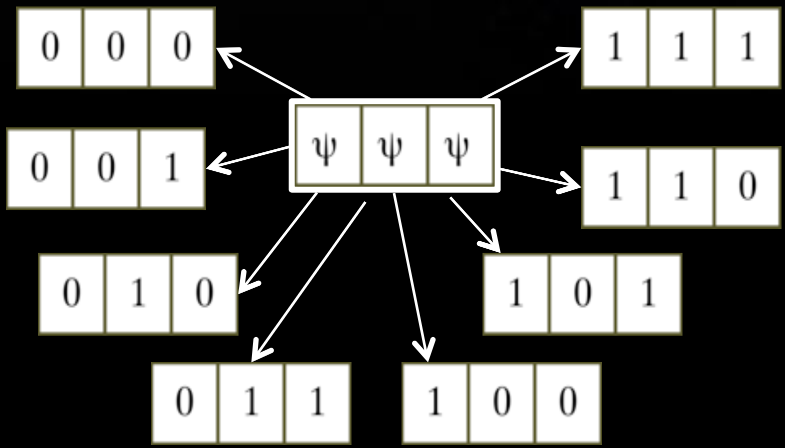
- Statistical downscaling of coarse data from CMIP5 (for IPCC) for conterminous U.S. to obtain high-resolution predictions at local scale
- ~800m grid resolution
- Spring (March–May), 1950–2099
- Mean temperature projected to increase from 12°C to 15°C assuming greenhouse gas emissions stabilize in 2050
- Area at or below 0°C isotherm decreases from 2.5M sq. km to 0.6M sq. km

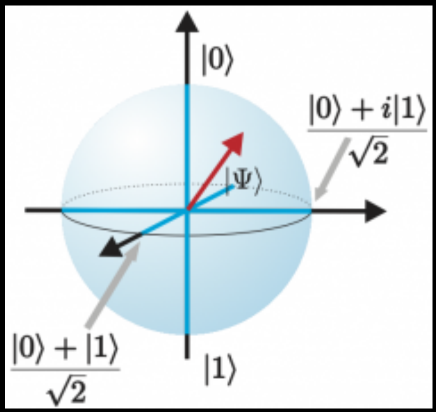


- Details in paper by B. Thrasher et al.: *"Downscaled climate projections suitable for resource management,"* Eos, Vol. 94, No. 37, Sept. 2013, pp. 321-323

Quantum Computing

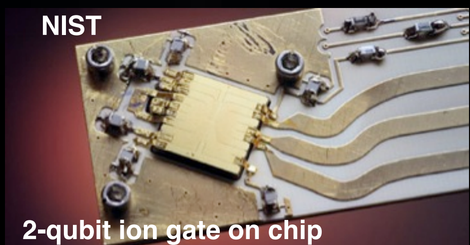
- Quantum mechanics deals with physical phenomena at very small scales (~100 nm) or at very low temperatures (few K) where actions are quantized
- The outcome of a quantum experiment is probabilistically associated both with what was done before the measurement and how the measurement was conducted
- Qubits (quantum bits) can exist in a superposition of states, allowing *n* qubits to represent 2^n states simultaneously
- At the end of a computation, on measurement, the system collapses into a classical state returning only one bit string as a possible solution

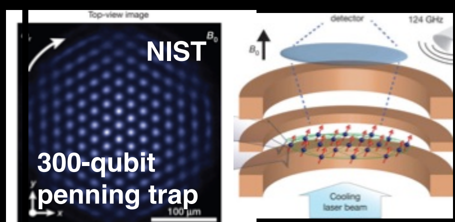




Quantum Computing Implementations

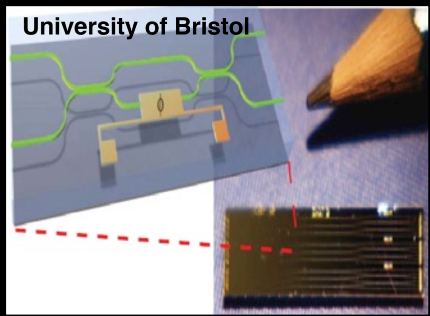
Trapped Ions and Trapped Neutral Atoms





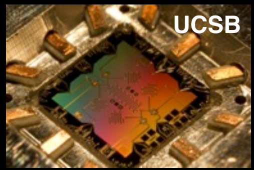
2-qubit ion trap with microwave control (top); 300-qubit ion trap in optical lattice (bottom)
(trapping and manipulation of ions and atoms)

Photonic Quantum Chips



4-qubit photonic chip with optical waveguides integrated in solid state
(position or polarization of photons used a qubit)

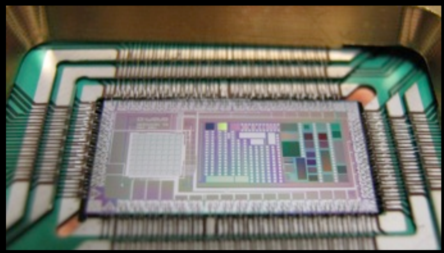
Superconducting Qubits



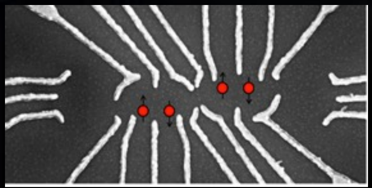
4-qubit universal quantum computing

D-WAVE "VESUVIUS"

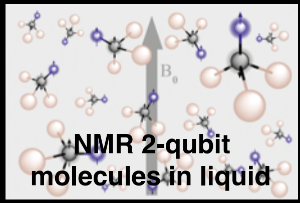
512-qubit – not universal

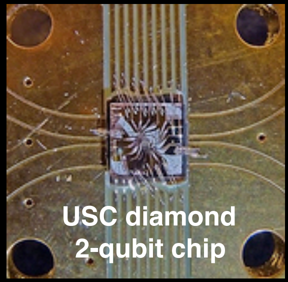


Nanoelectronics, NMR, Diamond Chips, …



RWTH Aachen 2-qubit gate



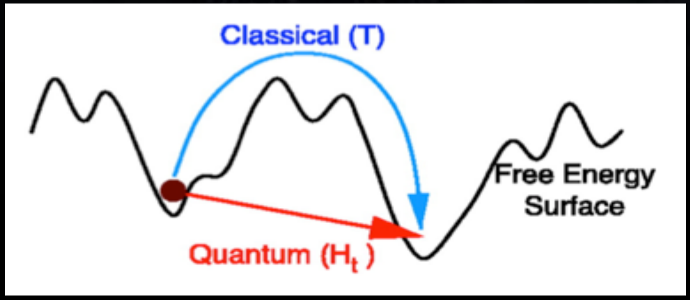


Quantum dots (top); spin states of molecules in liquid (middle); nitrogen vacancies in diamond (bottom)

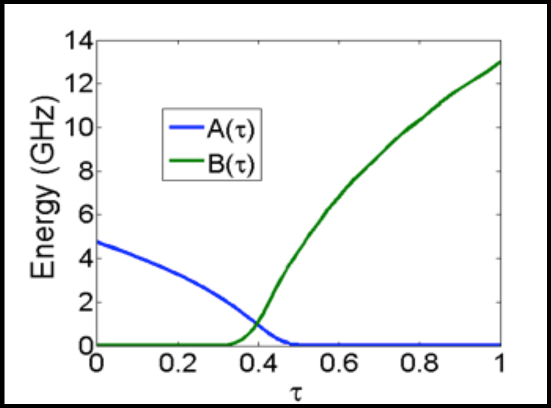
Quantum Annealing

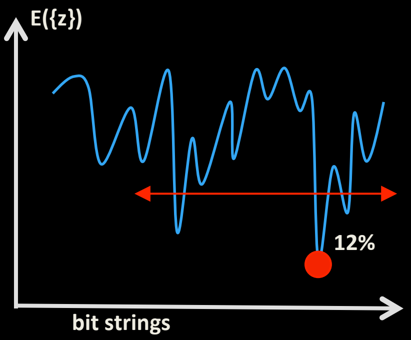
A physical technique to solve combinatorial optimization problems in QUBO (Quadratic Unconstrained Binary Optimization)

$$E(z_1, z_2, \dots z_n) = \underbrace{\left(1 - \frac{t}{T}\right)}_{A(t)} H_0(\{z\}) + \underbrace{\frac{t}{T}}_{B(t)} H_P(\{z\})$$

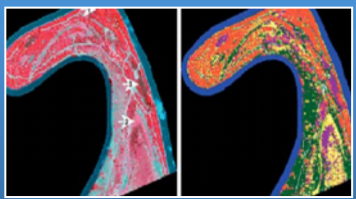


- *N*-bit string of unknown variables {*z*}
- H_0 : Hamiltonian with known ground state
- H_P: Hamiltonian whose ground state represents the solution to the problem
- *A(t)* is slowly (adiabatically) lowered to zero while maintaining minimum energy of the system at all times
- Solution is the configuration {*z*} that produces the minimum *E* with a non-zero probability



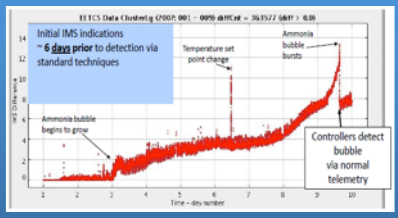


NASA and Quantum Computing

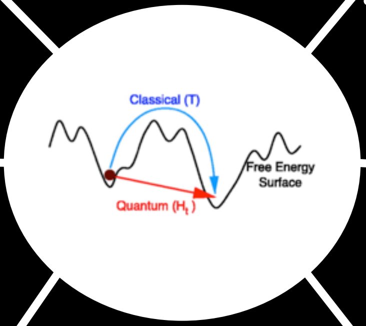


Data Analysis and Data Fusion

Anomaly Detection and Decision Making

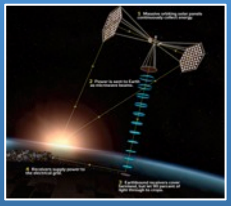


Air Traffic Management



V&V and optimal sensor placement

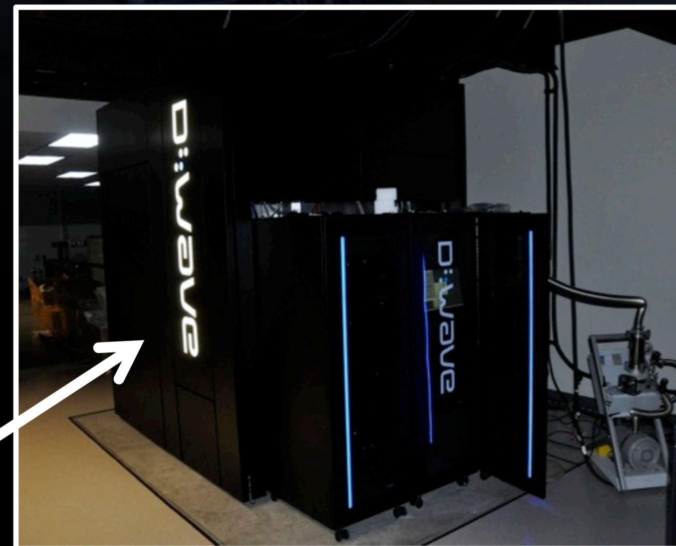
Mission Planning and Scheduling, and Coordination

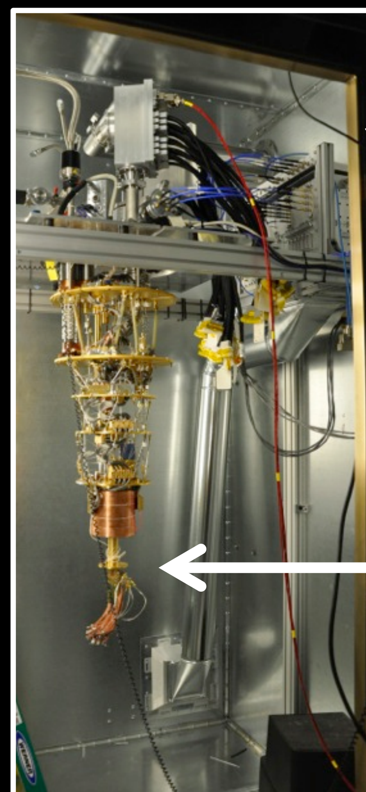


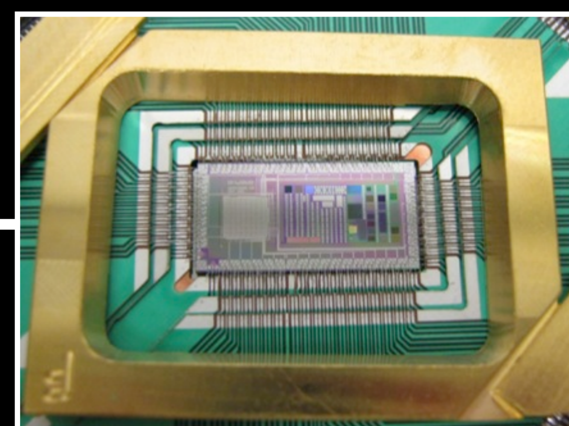
Topologically aware Parallel Computing

D-Wave Two System

- Collaboration among NASA, Google, and USRA led to installation of system at NAS Division
- 512-qubit Vesuvius processor (to be continuously upgraded over the next 4+ years)
- 10 kg of metal in vacuum at 15 mK
- Magnetic shielding to 1 nanoTesla
- Protected from transient vibrations
- Single run takes 20 μsecs
- Uses 12 kW of electrical power







Focused on solving discrete optimization problems using quantum annealing

Programming the D-Wave Two

1 Map the target combinatorial optimization problem into QUBO

No general algorithms, smart mathematical tricks (penalty functions, locality reduction..)

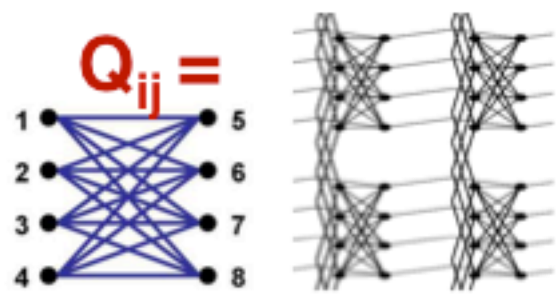
$$\alpha_{ijk} z_i z_j z_k$$

$$\alpha_{ijk} y_{ij} z_k + \beta_{ijk}(3y_{ij} - 2z_i y_{ij} - 2z_j y_{ij} + z_i z_j)$$

$$\sum_{ij} Q_{ij} z_i z_j$$

2 Embed the QUBO coupling matrix in the hardware graph of interacting qubits

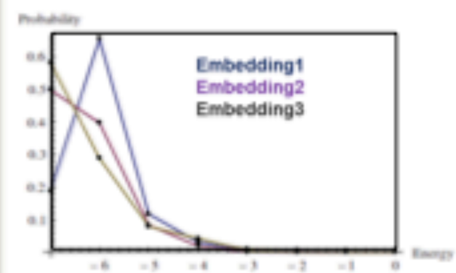
The D-Wave hardware qubit connectivity is a "Chimera Graph", so embedding methods mostly based on heuristics



Note: D-Wave provides a heuristic blackbox compiler that bypasses embedding

3 Run the problem many times and collect statistics

Use symmetries, permutations, and error correction to eliminate the systemic hardware errors and check the solutions



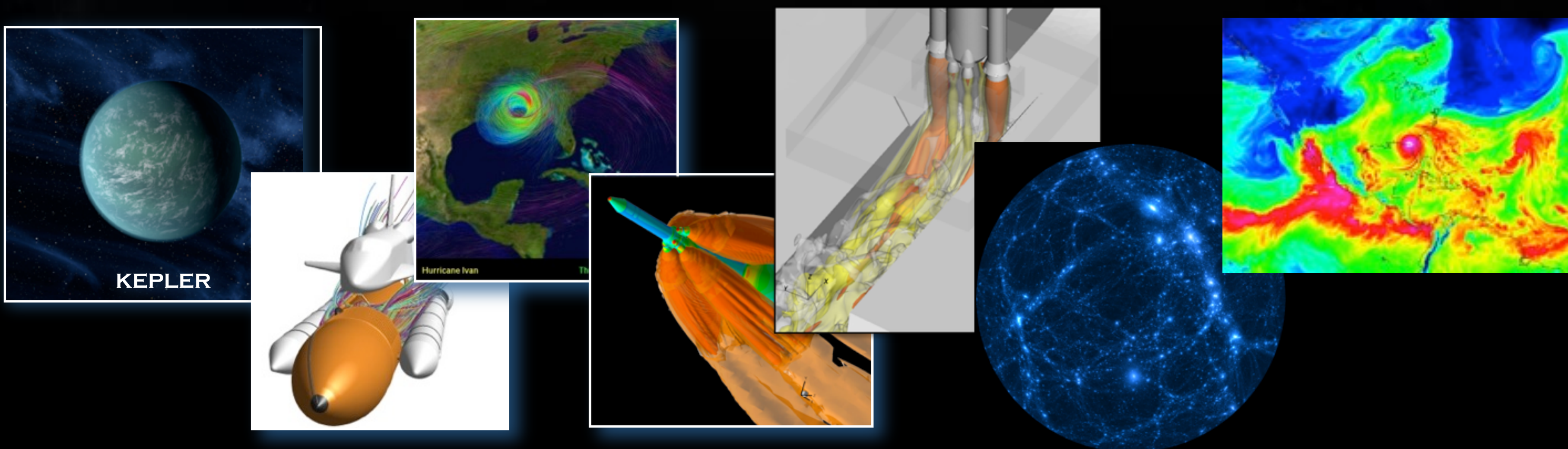
Mapping not needed for random spin-glass models

Embedding not needed for native Chimera problems

Performance can be improved dramatically with smart pre-/post-processing

Advanced Computing Mission

Enable the science & engineering required to meet NASA's missions and goals



Effective, stable, production-level HPC environment

Advanced technologies to meet future goals

Thank You!

Questions?

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